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EXTENDED ABSTRACT

INTRODUCTION To often the parallelism of a computational algorithm is used (or advertised) as a desirable measure of its performance. That is, the higher the computational parallelism the better the expected performance. With the current interest and emphasis on massively parallel computer systems, the notion of highly parallel algorithms is the subject of many conferences and funding proposals. Unfortunately, the "revolution" that this vision promises has served to further complicate the measure of parallel performance by the introduction of such notions as scaled speedup and scalable systems.

As a counter example to the merits of highly parallel algorithms whose parallelism scales linearly with increasing problem size, we introduce a slight modification to a highly parallel Monte Carlo technique that is used to estimate the solution of Poisson's equation. This simple modification is shown to yield a much better estimate to the solution by incorporating a more efficient use of boundary data (Dirichlet boundary conditions). A by product of this new algorithm is a much more efficient sequential algorithm but at the expense of sacrificing parallelism.

DESCRIPTION The two-dimensional Poisson equation with Dirichlet boundary conditions is given by:

$$\nabla^2 \phi(x,y) = \rho(x,y),$$
$$\phi(x_0,y_0) = f(x_0,y_0). \tag{1}$$

Although we consider only Dirichlet boundary conditions, the method may be extended to various other boundary conditions[1]. Using the five-point finite difference stencil, the discretized form of Eqn. (1) is given by

$$\phi_{ij} = \frac{1}{4}\left(\phi_{i-1,j} + \phi_{i,j-1} + \phi_{i+1,j} + \phi_{i,j+1} + \frac{\rho_{ij}}{h^2}\right). \tag{2}$$

Here, the spacing in x and y are both equal to some small grid spacing h.

Since the coefficients of the ϕ's of the points adjoining cell (i, j) sums to 1, each step may be thought of as the probability of taking a step from (i, j) to each of these cells, assuming equal probability to wander in each of the four directions. For this reason, a Monte Carlo estimate to the potential could be obtained by statistically sampling the solution domain by means of random walks that score the values of the boundary where they terminate. For non-zero ρ, one also scores the value of $\frac{\rho_{ij}}{4h^2}$ at every interior point (i, j) reached during the walk. This entails what is known as a "primary estimate" of the value of ϕ at point (i, j). For N primary estimates, the arithmetic mean of the N primary estimates gives the final estimate.

A standard Monte Carlo algorithm[2] used to estimate the solution of Poisson's equation at the point (i, j) requires a "particle" or "sample" to be initialized with its position being equal to the cell indices (i, j) and having two accumulators. One accumulator scores $\frac{\rho_{kl}}{4h^2}$ at each interior point (k, l) of the walk, the second scores the value of ϕ when the particle reaches a boundary. The interior tally is initialized with ρ at (I, j); the boundary tally is set to zero. As in other Monte Carlo simulations, the use of a pseudo-random number generator determines which of four possible directions the particle is to take for its "step". If the step takes the particle to an interior point, the accumulator for the charge density ρ is tallied at this point. The particle then continues its random walk from this point. If the new cell is a boundary point, the value of ϕ on the boundary is scored in the boundary tally and the particle history terminates. The tallies are multiplied by appropriate factors, giving an estimate for ϕ at this point. To achieve sufficient accuracy to the solution, a large number of particles are issued from point (I, j).

The expression for ϕ_{ij} is given as follows:

$$\phi_{I,J} \quad \sum_{n=1}^{N} \phi_{I(n),J(n)} + \frac{1}{4h^2} \sum_{n=1}^{N} \sum_{m=1}^{M(n)} \rho_{I'(n,m),J'(n,m)} \tag{3}$$

where N is the number of random walks started from (I, j), M(n) is the number of cells the N'th walk comprises, (I(n), J(n)) are the cell coordinates of the boundary on which the N'th walk terminates, and (I'(n, m), J'(n, m)) are the cell coordinates of the M'th cell through which the N'th walk passes.

One can understand the high degree of parallelism that is found in the standard Monte Carlo method if the approach is regarded as a Jacobi-like scheme where the estimate of each grid point within the solution domain is determined without reference to estimates obtained at other points. For this reason, the estimates of the solution at every point within the domain can proceed in parallel. This highly (massively) parallel approach was implemented

on the Intel iPSC/1-VX hypercube[3]. As a point of interest, we note that this implementation develops a computational load imbalance that arises from the variations in the number of random walks required for termination.

Disregarding the issue of performance measured in terms of absolute parallelism, a simple modification to the Jacobi-like Monte Carlo approach was developed that employs the efficient use of the (Dirichlet) boundary conditions to minimize both the number of random walks required to reach the boundary and the total number of particles required to obtain a comparable or better convergenced solution. The modified approach propagates the boundary information into the center of the solution domain. The procedure consists of initiating random walks from only those grid points next to the boundary. After all random walks from these grid points have terminated, the points themselves are taken as the new boundary points. The procedure continues in this manner until the boundary information is, in effect, propagated into the center of the solution domain. This boundary propagation method is a Gauss-Seidel like scheme and subsequently has less available computational parallelism. Since the random walks are issued from only those points closest to the boundary, the probability is very high that only a few steps are required to reach the boundary.

RESULTS For the test problem, the charge density on the right hand side of Poisson s equation was chosen to be

$$\rho(x,y) = \sin(x)\sin(y). \tag{4}$$

The convergence of the boundary propagation method was studied by running the test problem with different number of samples (or particles) per grid point. The estimated values of the potential was compared against a direct method based on the five point difference stencil. The test problems ran with mesh sizes of 34 x 34 and 66 x 66 (where the boundaries are included in the dimensions). Because of the differencing scheme used, the truncation error of order h^2 can clearly be distinguished between the solutions of the 34 x 34 and 66 x 66 cases. Since in the boundary propagation method, the longest random walks occur for thoses samples that start from the grid points adjacent to the original boundary, the total number of random walks required for termination within the entire solution domain is significantly less than the total number of random walks required by the highly parallel (Jacobi-like) method. For equivalent numbers of particles, we have measured execution times to be from 14 to 18 times faster for the boundary method as opposed to the first method. Furthermore for the same number of samples per grid point, the boundary propagation method achieved significantly better estimates of the solution. Further details of our results will be presented during the session.

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